MOMENTUM DENSITY OF HIGH T_c COPPER OXIDES

B. Barbiellini and P.M. Platzman

Bell Laboratories, Lucent Technologies, 700 Mountain Ave, Murray Hill, NJ 07974, USA

Keywords: high T_c superconductors, Compton profile, positron annihilation spectroscopy.

Abstract: We discuss the work aimed at studying the momentum density of high T_c superconducting oxides using Compton profile and positron annihilation spectroscopies.

Several experiments and theoretical models suggest that strong electron correlation effects are involved in the description of copper oxides [1]. While searching for the Fermi surface (FS), a more general question to ask is: What is the influence of strong correlations on the momentum density ? Unfortunately, the overall momentum density in such materials is described quite well by a local tight-binding description of the transition metal surrounded by, for example, an octahedron of oxygen atoms [2]. Thus the dominant features are due to wavefunctions effects, and the FS plays a minor role. Instructive examples of the importance of orbital contributions in momentum density are found from the 2D-ACAR (2-Dimensional Angular Correlation of the Annihilation Radiation) technique applied to copper oxides [3]. The momentum density anisotropies of $La_{2-x}Sr_xCuO_4$ [4, 5] and $Tl_{2-x}Ba_xCuO_6$ [6] can be described reasonably well by a simple LCAO-MO method [2], which neglects the FS. Therefore, in these cases the chemical bonding overshadows the smaller FS effects and it is very difficult to extract the FS signal. However, a more favorable case is provided by the $YBa_2Cu_3O_{7-\delta}$, where the 1-dimensional ridge FS has a two-fold symmetry which distinguishes it from important four-fold symmetry wave function effects [7]. Another important result obtained by the positron annihilation spectroscopy [8] is the observation of a ridge FS signal in the insulating $PrBa_2Cu_3O_{7-\delta}$. Therefore the insulating character of this compound can be explained by defects in the Cu-O chains, that prevent it from conducting, and by the existence a mechanism which binds the doped holes to the Pr sites, making the Cu-O planes insulating [9].

Several recent publications have suggested that the unusual features of the c-axis resistivities observed in the cuprates could be an indication of the non-Fermi-liquid nature of these materials [10]. For instance, the c-axis resistivities estimated from band theory are at least a factor of ten smaller than the experimental values. Moreover the standard band theory for 2-layer cuprates compounds [11, 12] predicts due to bonding antibonding states a two piece FS, while

photoemission results in $Bi_2Sr_2CaCu_2O_8$ do not show split Fermi surfaces [13]. However, the photoemission results do not yet rule out the Fermi-liquid theory, since they might also be explained by strong polarization selections rules.

Anderson, Clarke and coworkers [10, 14, 15] have suggested that coherent tunneling between the planes is forbidden because of an in-plane Fermi-liquid breakdown and that coherent pair tunneling becomes allowed when we enter the superconducting state. This argument remains controversial. We propose to look at the consequences of this assumption on the momentum density.

While positron annihilation is a possible technique, it presents some difficulties. In copper oxides the spatial distribution of the positron wave function has a large contribution on the 2D-ACAR spectra. For instance, in $YBa_2Cu_3O_{7-\delta}$ the positrons are mainly located along the Cu-O chains, while in $Nd_{2-x}Ce_xCuO_4$ they have more overlap with the Cu-O planes. Therefore, $Nd_{2-x}Ce_xCuO_4$ is a more suitable compound for probing the Cu-O planes with positrons [17]. Unfortunately the defects contained in the real samples make this investigation difficult, since they trap the positrons. Nevertheless a recent 2D-ACAR experiment [16] indicates evidence of a FS signal from the Cu-O layers.

Compared with positron annihilation, Compton scattering [18] offers some advantages. The results are not sensitive to sample purity or to lattice defects. Moreover the interpretation of the data is not complicated by the positron wave function and correlation effects. Nevertheless, the 2D-ACAR spectrum gives a projection of the momentum density along the direction perpendicular to the 2-dimensional detectors, whereas the Compton profile allows one only to identify structures in the momentum density averaged over the planes perpendicular to the scattering vector. Therefore, we can view these two spectroscopies as being complementary tools [19] to study the different pieces of the FS of the high T_c superconducting oxides. In the case of $YBa_2Cu_3O_{7-\delta}$, the 2D-ACAR has identified the ridge FS associated with the Cu-O chains, while the Compton scattering could be used for the study of the barrel portions of the FS, which are connected with the interlayer coupling.

The standard local density approximation (LDA) [11] predicts an energy splitting for 2-layer high T_c compounds, due to electron coherent motion between the layers. In $YBa_2Cu_3O_7$, where two neighboring Cu-O planes are separated by $d = 6.43$ (a.u.), the coherent motion between Cu-O planes would give a feature at $p = 2\pi/d$ in the Compton profile along the c axis. To detect this feature, one can consider differences of the directional Compton profiles along two directions: in plane and along the c-axis [20]. The LDA calculations give a structure in the differences of the directional Compton profiles [001]-[100] and [001]-[010] located at $p = 2\pi/d \approx 1$ (a.u.) (see Fig.1). We have simulated the effect of suppressed tunneling by shifting the Fermi energy an amount comparable to the energy separation of bonding and antibonding states. The amplitude of this modulation depends on the position of the Fermi level (or on the difference of electrons contained in the two Fermi surfaces of the Cu-O planes) and its predicted value is of the order

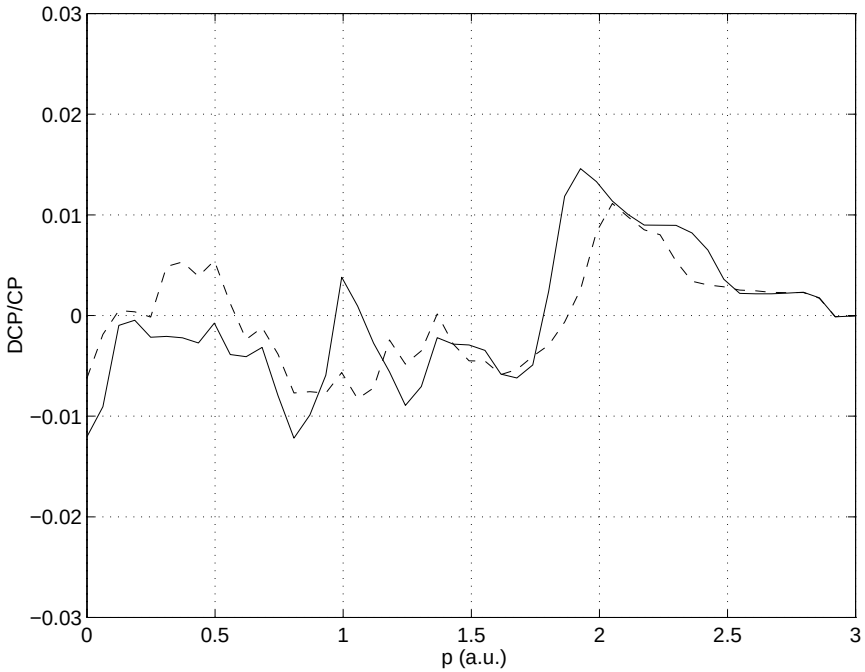

Figure 1: Directional differences of Compton profiles [001]-[100] for twinned $YBa_2Cu_3O_7$ as given by a band structure calculation. Full line: the peak near 1 a.u. is the structure mentioned in the text. Dashed line: the peak disappears by shifting the Fermi Energy by + 1.3 eV.

of 1%. Therefore it should be detectable with more than 10^4 counts in a resolution bin of 0.15 (a.u.). On the other hand, the absence of this signal, which implies a degenerate FS of the Cu-O planes, would be consistent with Anderson's suggestion.

A very important question regarding the nature of the electronic ground state of high T_C materials is the character of the extra holes introduced when we dope away from half filling. Experiments seem to show that the holes introduced by doping reside primarily on oxygen sites. The suggestion of Zhang and Rice [21] is that they reside in a molecular orbital state $P_{MO} = P_{1x} - P_{2y} - P_{3x} + P_{4y}$. The orbital P_{MO} couples with the Cu $3d_{x^2-y^2}$ state and forms a singlet named after Zhang and Rice [21].

The difference of the directional Compton profiles [100]-[110] should reflect anisotropy of the Cu ($3d_{x^2-y^2}$) holes (see Fig. 2A). P_{MO} gives an additional anisotropy. Its contribution (see Fig. 2B) is expected to increase with the doping. For an optimally doped sample, we expect there to be a 20-10 % increase of the anisotropy and an additional periodic structure which can be directly related to the phases of the wave function associated with the four oxygens surrounding a given Cu atom. However, positron annihilation experiments in $La_{2-x}Sr_xCuO_4$ [22] have not observed significant change in the shape of the anisotropies as a function of x. One possible explanation is that the Zhang-Rice singlet is a positive object which repels the positron. If so the Zhang-Rice singlets would not be seen by positron but may be observed in Compton scattering experiments.

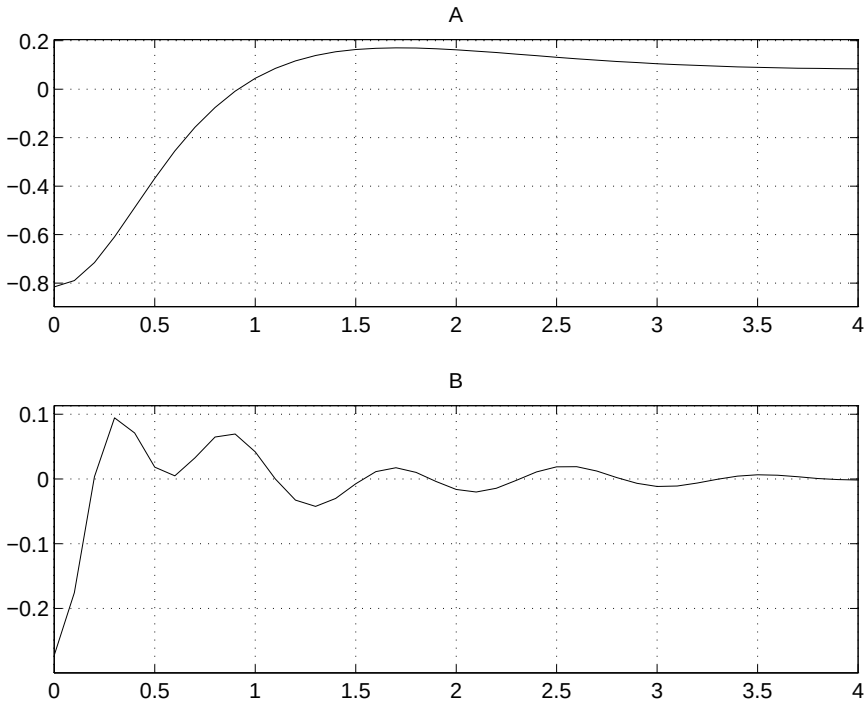

Figure 2: Directional differences of Compton profiles [100]-[001]. A: contribution of the Cu ($3d_{x^2-y^2}$) hole (arbitrary units). B: contribution of the P_{MO} hole for optimally doped sample.

In conclusion 2D-ACAR and Compton scattering high resolution momentum experiments are useful tools to probe the electronic structure of the high T_c superconducting oxides. By using these two spectroscopies we can gain insight into the question of the electron-electron correlations and of the FS.

Acknowledgements: We wish to thank A.A. Manuel, A. Shukla, T. Jarlborg, F.C. Zhang and E. Isaacs for discussions. B.B. was supported by the Swiss National Science Foundation Grant No. 8220-037167.

References

[1] E. Dagotto, Rev. Mod. Phys. **66** (1994) p. 763.

[2] T. Chiba, J. Chem. Phys. **64** (1976), p. 1182; T. Chiba, J. Phys. Chem. Solids **53** (1992), p. 1677.

[3] A.A. Manuel, A. Shukla, L. Hoffmann, T. Jarlborg, B. Barbiellini, S. Massidda, W. Sadowski, E. Walker, A. Erb and M. Peter, J. Phys. and Chem. of Solids **56** (1995), p. 1951.

[4] P.E.A. Turchi, A.L. Wachs, K.L. Wetzler, J.H. Kaiser, R.N. West, Y.C. Jean, R.H. Howell and M.J. Fluss, J. Phys. Condens. Matter **2** (1990), p. 1635.

[5] P.A. Sterne, R.H. Howell, M.J. Fluss, J.H. Kaiser, K. Kitazawa and H. Kojima, J. Phys. Chem. Solids **54**, (1993), p. 1231.

[6] B. Barbiellini, M. Gauthier, L. Hoffmann, T. Jarlborg, A.A. Manuel, S. Massidda, M. Peter and G. Triscone, Physica C **229** (1994), p. 113.

[7] H. Haghighi, J.H. Kaiser, S. Rayner, R. N. West, J.Z. Liu, R. Shelton, R. H. Howell, F. Solal and M. J. Fluss, Phys. Rev. Lett. **67** (1991), p. 382.

[8] L. Hoffmann, A.A. Manuel, M. Peter, E. Walker, M. Gauthier, A. Shukla, B. Barbiellini, S. Massidda, Gh. Adam, S. Adam, W.N. Hardy and Ruixing Liang, Phys. Rev. Lett. **71** (1993), p. 4047.

[9] R. Fehrenbacher and T.M. Rice, Phys. Rev. Lett. **70** (1993), p. 3471.

[10] D.G. Clarke, S.P. Strong and P.W. Anderson, Phys. Rev. Lett. **72** (1994), p. 3218.

[11] S. Massidda, J. Yu, A.J. Freeman and D.D. Koelling, Phys. Lett. A 122 (1987), p. 198.

[12] W.E. Pickett, Rev. Mod. Phys. **61** (1989), p. 433.

[13] Z.X. Shen and D.S. Dessau, Phys. Report **253** (1995), p. 72.

[14] P. W. Anderson and J. R. Schrieffer, Physics Today, June (1991), p. 54.

[15] S. Chakravarty, A. Subdø, P.W. Anderson and S. Strong, Science **261** (1993) p. 33.

[16] A. Shukla, B. Barbiellini, L. Hoffmann, A. A. Manuel, W. Sadowski, E. Walker and M. Peter, Phys. Rev. B **53** (1996), p. 3613.

[17] B. Barbiellini, M. J. Puska, A. Harju and R.M. Nieminen, J. Phys. and Chem. of Solids **56** (1995), p. 1693.

[18] E. D. Isaacs and P.M. Platzman, Physics Today, February (1996), p. 40.

[19] L.C. Smedskjaer and A. Bansil, Z. Naturforsh. **48 a** (1992), p. 398.

[20] P.M. Platzman, F.C. Zhang, E. Isaacs, B. Barbiellini, A. Shukla, A.A. Manuel, A. Erb, experiment proposal at ESRF.

[21] F.C. Zhang and T.M. Rice, Phys. Rev. B **37** (1988) p. 3759.

[22] R.H. Howell, P.A. Sterne, M.J. Fluss, J.H. Kaiser, K. Kitazawa, H. Kojima, Phys. Rev. B **49** (1994), p. 13127.